

Propaneperoxoic acid, 2-methyl-, 1,1-dimethylethyl ester
109-13-7 | DTXSID1059363

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 45.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 7.22e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N-Methyl-N'-phenylurea</div> <div>Measured: 19.5</div> <div>Predicted: 29.8</div>	<div>Image not found</div> <div>Urea, (3-methylphenyl)-</div> <div>Measured: 36.3</div> <div>Predicted: 37.2</div>	<div>Image not found</div> <div>N-Acetyl-m-toluidine</div> <div>Measured: 28.2</div> <div>Predicted: 42.1</div>
<div>Image not found</div> <div>Methyl phenylcarbamate</div> <div>Measured: 53.7</div> <div>Predicted: 59.1</div>	<div>Image not found</div> <div>Ethyl benzoate</div> <div>Measured: 200</div> <div>Predicted: 97.1</div>	